

Note to readers with disabilities: *EHP* strives to ensure that all journal content is accessible to all readers. However, some figures and Supplemental Material published in *EHP* articles may not conform to [508 standards](#) due to the complexity of the information being presented. If you need assistance accessing journal content, please contact ehp508@niehs.nih.gov. Our staff will work with you to assess and meet your accessibility needs within 3 working days.

Supplemental Material

Evaluation of OASIS QSAR Models Using ToxCast *in Vitro* Estrogen and Androgen Receptor Binding Data and Application in an Integrated Endocrine Screening Approach

Barun Bhattacharai, Daniel M. Wilson, Paul S. Price, Sue Marty, Amanda K. Parks, and Edward Carney

Table of Contents

Table 1. Details for the ToxCast ER and AR binding and transactivation assays selected during 3D-QSAR based prediction study

Excel File, Table 2a. See “Additional Files” below

Table 2b. Summary performance of QSAR model predictions for **all** ToxCast II compounds against individual mammalian *in vitro* assays for Estrogen Receptor (ER) binding model v.03 (top) and Androgen Receptor (AR) binding model v.03 (bottom).

Table 3a. Summary performance of QSAR model predictions for all 42 and 36 in-domain compounds with uterotrophic bioactivity

Table 3b. Eleven compounds that have ER binding at $AC_{50} < 1 \mu M$ for all the three mammalian nuclear receptor binding assays were also active in the uterotrophic assay. They also belong to the training set data used to derive the ER QSAR model. The *in silico* prediction results including the total domain information as well as *in vitro* assay data are given

Table 3c. Four compounds (3 Phthalates and 1 Kaempferol) belonging to the training set were considered active in the ER *in vitro* assay used to derive the model but where inactive in uterotrophic bioactivity

Table 4a. Sixteen compounds that were active experimentally and belonged to the training set but were predicted not active for ER binding

Table 4b. Fifteen Compounds that were not active experimentally and belonged to the training set but were predicted active for ER binding

Table 5a. Twelve compounds that were active experimentally and belonged to the training set but were predicted not active for AR binding

Table 5b. Two compounds that were not active experimentally and belonged to the training set but were predicted active for AR binding

Additional Files

Supplemental Code and Data Zip File

Supplemental Code and Data Zip File Index

Excel File, Table 2a. The total chemical lists, CAS numbers, SMILES codes, corresponding ToxCast assay values, potency bins, and calculated RBA values